

I U C L I D

Data Set

Existing Chemical : ID: 3757-76-4
CAS No. : 3757-76-4
Generic name : 2,4-Dichlorophenol sodium salt

Producer Related Part
Company : The Dow Chemical Company
Creation date : 24.01.2002

Substance Related Part
Company : The Dow Chemical Company
Creation date : 24.01.2002

Memo :

Printing date : 25.01.2002
Revision date :
Date of last Update : 25.01.2002

Number of Pages : 4

Chapter (profile) :
Reliability (profile) :
Flags (profile) : ???

1.0.1 OECD AND COMPANY INFORMATION

Type : cooperating company
Name : The Dow Chemical Company
Partner :
Date :
Street : 2020 Dow Center
Town : 48674 Midland, Michigan
Country : United States
Phone :
Telefax :
Telex :
Cedex :
25.01.2002

1.0.2 LOCATION OF PRODUCTION SITE**1.0.3 IDENTITY OF RECIPIENTS****1.1 GENERAL SUBSTANCE INFORMATION****1.1.0 DETAILS ON TEMPLATE****1.1.1 SPECTRA****1.2 SYNONYMS****1.3 IMPURITIES****1.4 ADDITIVES****1.5 QUANTITY****1.6.1 LABELLING****1.6.2 CLASSIFICATION****1.7 USE PATTERN**

1.7.1 TECHNOLOGY PRODUCTION/USE**1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES****1.9 SOURCE OF EXPOSURE****1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES****1.10.2 EMERGENCY MEASURES****1.11 PACKAGING****1.12 POSSIB. OF RENDERING SUBST. HARMLESS****1.13 STATEMENTS CONCERNING WASTE****1.14.1 WATER POLLUTION****1.14.2 MAJOR ACCIDENT HAZARDS****1.14.3 AIR POLLUTION****1.15 ADDITIONAL REMARKS****1.16 LAST LITERATURE SEARCH****1.17 REVIEWS****1.18 LISTINGS E.G. CHEMICAL INVENTORIES**

2.1 MELTING POINT

Decomposition : yes at = 305 ° C
Sublimation :
Method : OECD Guide-line 102 "Melting Point/Melting Range"
Year : 2002
GLP : yes
Test substance : other TS
Test substance : 99.9% purity
Reliability : (1) valid without restriction
25.01.2002

(1)

2.2 BOILING POINT

Decomposition : yes
Method : OECD Guide-line 103 "Boiling Point/boiling Range"
Year : 2002
GLP : yes
Test substance : other TS
Test substance : 99.9% Purity
Reliability : (1) valid without restriction
25.01.2002

(2)

2.3 DENSITY**2.3.1 GRANULOMETRY****2.4 VAPOUR PRESSURE**

Value : < .0000000002 hPa at 20° C
Decomposition : no
Method : other (calculated)
Year : 2002
GLP : yes
Test substance : other TS
Decomposition : no
Test substance : 99.9% purity
Reliability : (1) valid without restriction
25.01.2002

(2)

2.5 PARTITION COEFFICIENT

Log pow : = .12 at 20° C
Method : other (calculated)
Year : 2002
GLP : yes
Test substance : other TS
Test substance : 99.9% purity
Reliability : (1) valid without restriction
25.01.2002

(1)

2.6.1 WATER SOLUBILITY

Value : = 6.04 g/l at 20 ° C
Qualitative : of high solubility
Pka : 7.8 at 25 ° C
PH : = 4 at and ° C
Method : OECD Guide-line 105 "Water Solubility"
Year : 2002
GLP : yes
Test substance : other TS
Remark : pKa is same as noted for 2,4-dichlorophenol.
Result : Water Solubility (at 20 C)

pH 4= 6.04 g/L
pH 7= 7.05 g/L
pH 10= 142 g/L
Unbuffered > 500 g/L

As evident by the high water solubility in unbuffered water (>500 g/L) and as expected for a salt (by definition), the test substance completely dissociates in water.

Therefore, the acid dissociation constant (pKa) for sodium salt of 2,4-dichlorophenol is the same as for 2,4-dichlorophenol.

Test substance : 99.9% purity
Reliability : (1) valid without restriction
25.01.2002

(1)

2.6.2 SURFACE TENSION**2.7 FLASH POINT****2.8 AUTO FLAMMABILITY****2.9 FLAMMABILITY****2.10 EXPLOSIVE PROPERTIES****2.11 OXIDIZING PROPERTIES****2.12 ADDITIONAL REMARKS**

3.1.1 PHOTODEGRADATION**3.1.2 STABILITY IN WATER****3.1.3 STABILITY IN SOIL****3.2 MONITORING DATA****3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS****3.3.2 DISTRIBUTION****3.4 MODE OF DEGRADATION IN ACTUAL USE****3.5 BIODEGRADATION****3.6 BOD5, COD OR BOD5/COD RATIO****3.7 BIOACCUMULATION****3.8 ADDITIONAL REMARKS**

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO₃), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO₃ in equilibrium with the atmosphere (pCO₂=3x10⁻⁴ atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water (Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability : (1) valid without restriction

25.01.2002

(3) (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Method :
Year : 2002
GLP :
Test substance :
Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to

range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO₃), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO₃ in equilibrium with the atmosphere (pCO₂=3x10⁻⁴ atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water (Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability

25.01.2002

: (1) valid without restriction

(3) (4)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE**Method**

:

Year

: 2002

GLP

:

Test substance

:

Remark

:

2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO₃), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO₃ in equilibrium with the atmosphere (pCO₂=3x10⁻⁴ atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water

(Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability

25.01.2002

: (1) valid without restriction

(3) (4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA**4.5.1 CHRONIC TOXICITY TO FISH****4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES****4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS****4.6.2 TOXICITY TO TERRESTRIAL PLANTS****4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES****4.7 BIOLOGICAL EFFECTS MONITORING****4.8 BIOTRANSFORMATION AND KINETICS****4.9 ADDITIONAL REMARKS**

5.1.1 ACUTE ORAL TOXICITY**5.1.2 ACUTE INHALATION TOXICITY****5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES****5.2.1 SKIN IRRITATION****5.2.2 EYE IRRITATION****5.3 SENSITIZATION****5.4 REPEATED DOSE TOXICITY****5.5 GENETIC TOXICITY 'IN VITRO'****5.6 GENETIC TOXICITY 'IN VITRO'****5.7 CARCINOGENITY****5.8 TOXICITY TO REPRODUCTION****5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY****5.10 OTHER RELEVANT INFORMATION****5.11 EXPERIENCE WITH HUMAN EXPOSURE**

- (1) Unpublished data, Dow Agrosciences LLC.
- (2) Unpublished data, Dow Agrosciences LLC
- (3) Allison, J.D., D.S. Brown and K.S. Novo-Gradac. 1991. MINTEQA2/PRODEFA2: A Geochemical Assessment Model for Environmental Systems. EPA/600/3-91/021. Assessment Branch, Environmental Research Laboratory, Athens, GA, USA.
- (4) Stumm, W. and J.J. Morgan. 1981. Aquatic Chemistry: An Introduction Emphasizing Chemical Equilibria in Natural Waters, 2nd Edition. John Wiley and Sons, Inc. New York. p. 183.

7.1 END POINT SUMMARY

Chapter : 4

Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO₃), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO₃ in equilibrium with the atmosphere (pCO₂=3x10⁻⁴ atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water (Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability : (1) valid without restriction
25.01.2002

Chapter : 5

Remark : The solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations likely to be encountered in mammalian testing. Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in the mammalian intestinal tract, the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, mammalian toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability : (1) valid without restriction

25.01.2002

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT